Chemistry Research

At Philip Morris USA Research Center, Richmond, Virginia (right), scientists are using a NASA-developed computer program in a study of basic chemistry, a relatively new use of computer software.

They are studying the chemical reactions of burning, which is not the fairly simple process it is generally thought to be. Cellulose and other complex polysaccharides, for example, are capable of decomposing into a variety of smaller molecules as they burn, and these smaller molecules can combine with each other in many ways. These different options are called "reaction pathways."

Combustion reaction pathways have been mapped for many small and simple molecules, but larger molecules—like cellulose—are much more complicated; they break down into many different basic compounds when subjected to various burning conditions and thus are more difficult to study. The complex reaction pathways of these larger molecules are the focus of the Philip Morris study.

In order to gain insight into the behavior of atoms as they progress along the reaction pathway, Philip Morris scientists use a computer program called CECTRP, for Chemical Equilibrium Composition and Transport Properties. Originally developed by Lewis Research Center to model rocket fuel combustion, CECTRP was supplied to Philip Morris by NASA's Computer Software Management and Information Center (see page 122).

Use of the program lets the scientists predict accurately the behavior of a given molecule or a group of molecules. The computer-generated data must, of course, be checked by laboratory experiment, but the use of CECTRP saves the researchers hundreds of hours of laboratory time, since experiments must be run only to validate the computer's predictions, not to test each variable condition. Thus, CECTRP provides savings in experiment supplies and manpower while enabling scientists to test more ideas in a shorter period of time. In addition, Philip Morris estimates that, had CECTRP not been available, at least two man-years would have been required to develop a program to perform similar free energy calculations. ▲